Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials

Me-graphane: tailoring the structural and electronic properties of Me-graphene via hydrogenation

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I. ORBITAL PROJECTED BAND STRUCTURES

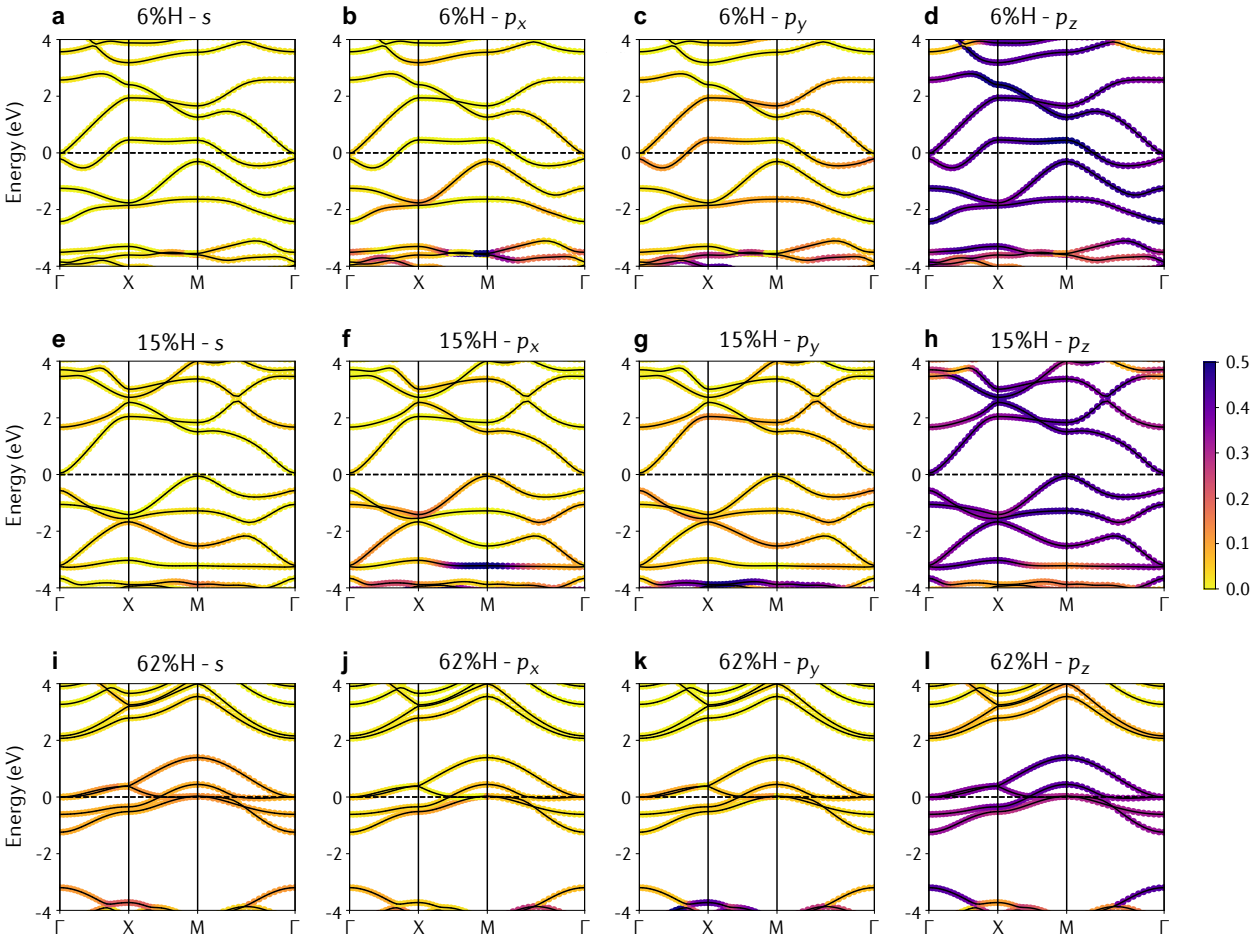

FIG. S1. Orbital-resolved band structures for (a-d) 6%, (e-h) 15%, and (i-l) 62%-hydrogenated Me-graphene (the scale indicates the magnitude of the projection). The orbitals s, p_x, p_y and p_z are projected onto the electronic bands. The zero energy is the Fermi level.

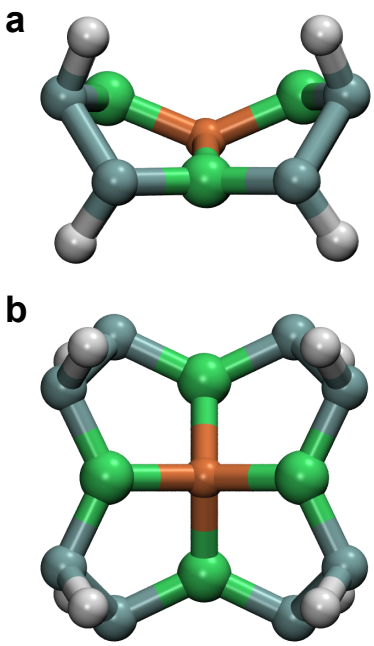

FIG. S2. Relaxed structure of 62%-hydrogenated Me-graphene: (a) side and (b) top view. We describe three carbon-atom sites: C_1 (sp^3) in orange, $C_2/C_{2'}$ (sp^2) in green and $C_3/C_{3'}$ (sp^2) in blue.

II. REACTIVE MOLECULAR DYNAMICS

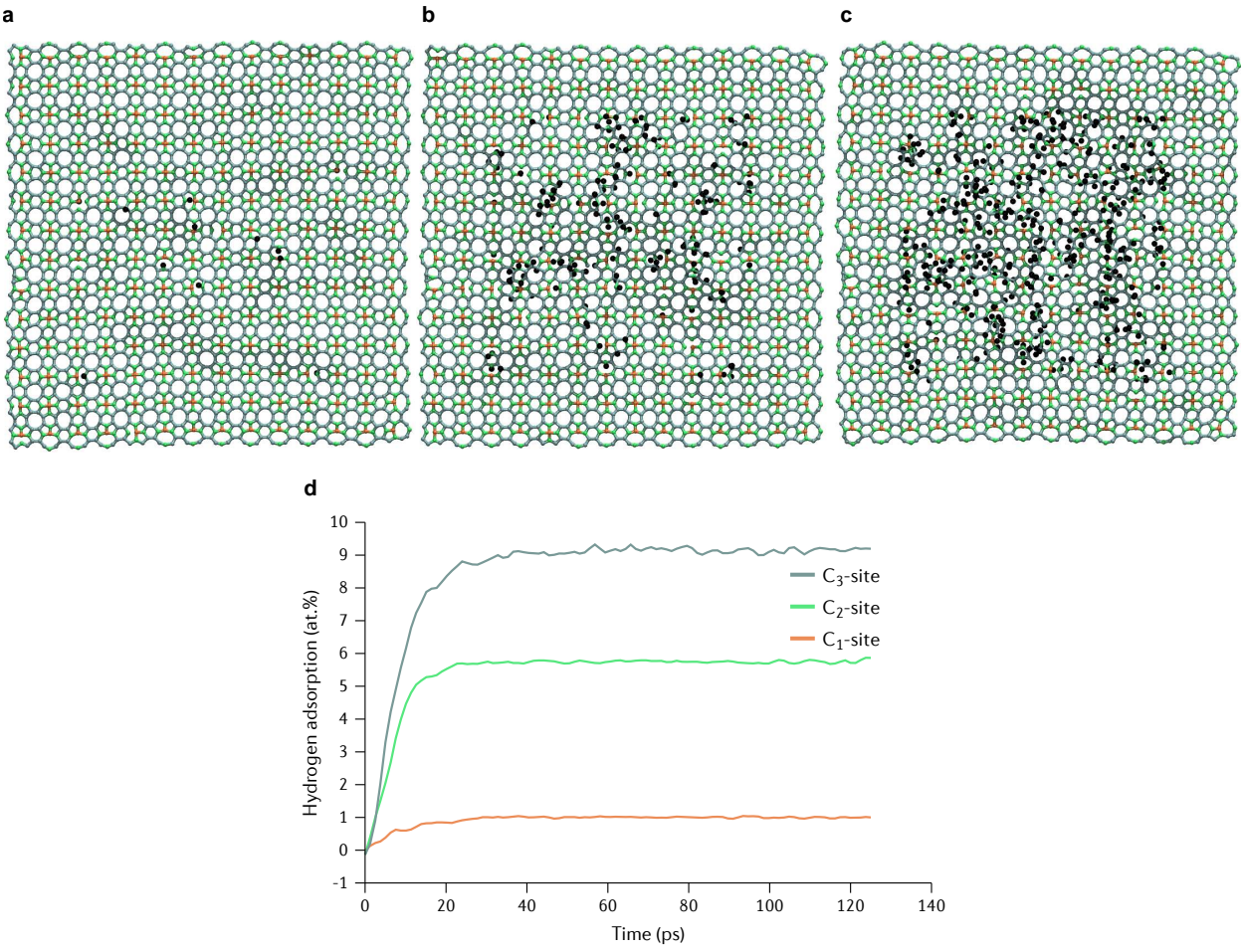

FIG. S3. Representative snapshots from the reactive molecular dynamics simulations of hydrogen incorporation process, where black spheres represent H atoms. (a) Early stage, (b) intermediate stage, and (c) final stage of the H adsorption dynamics at 800 K. (d) Hydrogen adsorption rate in atomic percent as a function of reaction time at 800 K, regarding the adsorption sites C_1, C_2, and C_3.